

Package ‘PFIM’

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Type Package

Title Population Fisher Information Matrix

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NeedsCompilation no

Description Evaluate or optimize designs for nonlinear mixed effects models using the Fisher Information matrix. Methods used in the package refer to
Mentré F, Mallet A, Baccar D (1997) <[doi:10.1093/biomet/84.2.429](https://doi.org/10.1093/biomet/84.2.429)>,
Retout S, Comets E, Samson A, Mentré F (2007) <[doi:10.1002/sim.2910](https://doi.org/10.1002/sim.2910)>,
Bazzoli C, Retout S, Mentré F (2009) <[doi:10.1002/sim.3573](https://doi.org/10.1002/sim.3573)>,
Le Nagard H, Chao L, Tenaillon O (2011) <[doi:10.1186/1471-2148-11-326](https://doi.org/10.1186/1471-2148-11-326)>,
Combes FP, Retout S, Frey N, Mentré F (2013) <[doi:10.1007/s11095-013-1079-3](https://doi.org/10.1007/s11095-013-1079-3)> and
Seurat J, Tang Y, Mentré F, Nguyen TT (2021) <[doi:10.1016/j.cmpb.2021.106126](https://doi.org/10.1016/j.cmpb.2021.106126)>.

URL <http://www.pfim.biostat.fr/>, <https://github.com/packagePFIM>

BugReports <https://github.com/packagePFIM/PFIM/issues>

Depends R (>= 4.0.0)

License GPL (>= 3)

Encoding UTF-8

VignetteBuilder knitr

Imports utils, inline, Deriv, methods, deSolve, purrr, stringr, S7,
Matrix, ggplot2, Rcpp, RcppArmadillo, pracma, kableExtra,
tibble, scales, knitr

Collate 'Administration.R' 'AdministrationConstraints.R' 'Fim.R'
'PFIMProject.R' 'Optimization.R' 'PGBAlgorithm.R'
'PSOAlgorithm.R' 'SimplexAlgorithm.R' 'FedorovWynnAlgorithm.R'
'MultiplicativeAlgorithm.R' 'Model.R' 'Arm.R' 'BayesianFim.R'
'ModelError.R' 'Combined1.R' 'Constant.R' 'Design.R'
'Distribution.R' 'Evaluation.R' 'IndividualFim.R'
'LibraryOfModels.R' 'LibraryOfPDModels.R' 'LibraryOfPKModels.R'
'LogNormal.R' 'ModelODE.R' 'ModelAnalytic.R' 'ModelInfusion.R'

'ModelAnalyticInfusion.R' 'ModelAnalyticInfusionSteadyState.R'
 'ModelAnalyticSteadyState.R' 'ModelODEBolus.R'
 'ModelODEDoseInEquations.R' 'ModelODEDoseNotInEquations.R'
 'ModelODEInfusion.R' 'ModelODEInfusionDoseInEquation.R'
 'ModelParameter.R' 'Normal.R' 'PFIM-package.R'
 'PopulationFim.R' 'Proportional.R' 'SamplingTimeConstraints.R'
 'SamplingTimes.R' 'zzz.R'

RoxygenNote 7.3.3

Suggests rmarkdown, testthat (>= 3.0.0)

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PFIM-package	<i>Fisher Information matrix for design evaluation/optimization for non-linear mixed effects models.</i>
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Description

Evaluate or optimize designs for nonlinear mixed effects models using the Fisher Information matrix. Methods used in the package refer to Mentré F, Mallet A, Baccar D (1997) [doi:10.1093/biomet/84.2.429](https://doi.org/10.1093/biomet/84.2.429), Retout S, Comets E, Samson A, Mentré F (2007) [doi:10.1002/sim.2910](https://doi.org/10.1002/sim.2910), Bazzoli C, Retout S, Mentré F (2009) [doi:10.1002/sim.3573](https://doi.org/10.1002/sim.3573), Le Nagard H, Chao L, Tenaillon O (2011) [doi:10.1186/1471214811326](https://doi.org/10.1186/1471214811326), Combes FP, Retout S, Frey N, Mentré F (2013) [doi:10.1007/s11095-01310793](https://doi.org/10.1007/s11095-01310793) and Seurat J, Tang Y, Mentré F, Nguyen TT (2021) [doi:10.1016/j.cmpb.2021.106126](https://doi.org/10.1016/j.cmpb.2021.106126).

Description

Nonlinear mixed effects models (NLMEM) are widely used in model-based drug development and use to analyze longitudinal data. The use of the "population" Fisher Information Matrix (FIM) is a good alternative to clinical trial simulation to optimize the design of these studies. The present version, ****PFIM 7.0****, is an R package that uses the S4 object system for evaluating and/or optimizing population designs based on FIM in NLMEMs.

This version of ****PFIM**** now includes a library of models implemented also using the object oriented system S4 of R. This library contains two libraries of pharmacokinetic (PK) and/or pharmacodynamic (PD) models. The PK library includes model with different administration routes (bolus, infusion, first-order absorption), different number of compartments (from 1 to 3), and different types of eliminations (linear or Michaelis-Menten). The PD model library, contains direct immediate models (e.g. Emax and Imax) with various baseline models, and turnover response models. The PK/PD models are obtained with combination of the models from the PK and PD model libraries. ****PFIM**** handles both analytical and ODE models and offers the possibility to the user to define his/her own model(s). In ****PFIM 7.0****, the FIM is evaluated by first order linearization of the model assuming a block diagonal FIM as in Mentré et al. (1997). The Bayesian FIM is also available to give shrinkage predictions (Combes et al., 2013). ****PFIM 7.0**** includes several algorithms to conduct design optimization based on the D-criterion, given design constraints: the simplex algorithm (Nelder-Mead) (Nelder & Mead, 1965), the multiplicative algorithm (Seurat et al., 2021), the Fedorov-Wynn algorithm (Fedorov, 1972), PSO (*Particle Swarm Optimization*) and PGBO (*Population Genetics Based Optimizer*) (Le Nagard et al., 2011).

Documentation

Documentation and user guide are available at <http://www.pfim.biostat.fr/>

Validation

PFIM 7.0 also provides quality control with tests and validation using the evaluated FIM to assess the validity of the new version and its new features. Finally, **PFIM 7.0** displays all the results with both clear graphical form and a data summary, while ensuring their easy manipulation in R. The standard data visualization package `ggplot2` for R is used to display all the results with clear graphical form (Wickham, 2016). A quality control using the D-criterion is also provided.

Organization of the source files in the ‘/R’ folder

PFIM 7.0 contains a hierarchy of S4 classes with corresponding methods and functions serving as constructors. All of the source code related to the specification of a certain class is contained in a file named `[Name_of_the_class]-Class.R`. These classes include:

1. all roxygen `@include` to insure the correctly generated collate for the DESCRIPTION file,
2. a description of purpose and slots of the class,
3. specification of an initialize method,
4. all getter and setter, respectively returning attributes of the object and associated objects.

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References

- Dumont C, Lestini G, Le Nagard H, Mentré F, Comets E, Nguyen TT, et al. PFIM 4.0, an extended R program for design evaluation and optimization in nonlinear mixed-effect models. *Comput Methods Programs Biomed.* 2018;156:217-29.
- Chambers JM. Object-Oriented Programming, Functional Programming and R. *Stat Sci.* 2014;29:167-80.
- Mentré F, Mallet A, Baccar D. Optimal Design in Random-Effects Regression Models. *Biometrika.* 1997;84:429-42.
- Combes FP, Retout S, Frey N, Mentré F. Prediction of shrinkage of individual parameters using the Bayesian information matrix in nonlinear mixed effect models with evaluation in pharmacokinetics. *Pharm Res.* 2013;30:2355-67.
- Nelder JA, Mead R. A simplex method for function minimization. *Comput J.* 1965;7:308-13.
- Seurat J, Tang Y, Mentré F, Nguyen, TT. Finding optimal design in nonlinear mixed effect models using multiplicative algorithms. *Computer Methods and Programs in Biomedicine*, 2021.
- Fedorov VV. *Theory of Optimal Experiments*. Academic Press, New York, 1972.
- Eberhart RC, Kennedy J. A new optimizer using particle swarm theory. *Proc. of the Sixth International Symposium on Micro Machine and Human Science, Nagoya*, 4-6 October 1995, 39-43.
- Le Nagard H, Chao L, Tenaillon O. The emergence of complexity and restricted pleiotropy in adapting networks. *BMC Evol Biol.* 2011;11:326.

Wickham H. ggplot2: Elegant Graphics for Data Analysis, Springer-Verlag New York, 2016.

See Also

Useful links:

- <http://www.pfim.biostat.fr/>
- <https://github.com/packagePFIM>
- Report bugs at <https://github.com/packagePFIM/PFIM/issues>

adjustGradient	<i>adjustGradient: adjust the gradient for the log normal distribution.</i>
----------------	---

Description

adjustGradient: adjust the gradient for the log normal distribution.

Arguments

distribution	An object Distribution giving the distribution.
gradient	The gradient of the model responses.

Value

The adjusted gradient of the model responses.

Administration	<i>Administration</i>
----------------	-----------------------

Description

The class Administration represents the administration and stores information concerning the administration for the dosage regimen.

Usage

```
Administration(
  outcome = character(0),
  timeDose = numeric(0),
  dose = numeric(0),
  Tinf = numeric(0),
  tau = 0
)
```

Arguments

outcome	A string giving the outcome for the administration.
timeDose	A vector of double giving the time doses.
dose	A vector of double giving the doses.
Tinf	A vector of double giving the time for infusion Tinf.
tau	An integer giving the tau value for repeated dose or steady state.

AdministrationConstraints

AdministrationConstraints

Description

The class AdministrationConstraints represents the constraint of an input to the system. The class stores information concerning the constraints for the dosage regimen.

Usage

```
AdministrationConstraints(outcome = character(0), doses = list())
```

Arguments

outcome	A string giving the outcome for the administration.
doses	A vector of double giving the doses.

Arm

Arm

Description

The class Arm represents an arm and stores information concerning an arm.

Usage

```
Arm(
  name = character(0),
  size = numeric(0),
  administrations = list(),
  initialConditions = list(),
  samplingTimes = list(),
  administrationsConstraints = list(),
  samplingTimesConstraints = list(),
  evaluationModel = list(),
  evaluationGradients = list(),
  evaluationVariance = list(),
  evaluationFim = Fim()
)
```


Arguments

name	A string giving the name of the arm.
size	A integer giving the size of the arm.
administrations	A list giving the objects of class Administration that define the administrations of the arm.
initialConditions	A list giving the initial conditions for the ode model where the names are string that define the variable and their value are giving by double
samplingTimes	A list giving the objects of class SamplingTime that define the sampling time of the arm.
administrationsConstraints	A list giving the objects of class AdministrationsConstraints that define the administration constraints of the arm.
samplingTimesConstraints	A list giving the objects of class SamplingTimeConstraints that define the sampling time constraints of the arm.
evaluationModel	A list giving the evaluation of the responses of the arm.
evaluationGradients	A list giving the evaluation of the responses gradient of the arm.
evaluationVariance	A list giving the evaluation of the variance.
evaluationFim	A object of class Fim giving the Fisher Information Matrix.

armAdministration	<i>getArmAdministration: get the administration parameters of an arm.</i>
-------------------	---

Description

getArmAdministration: get the administration parameters of an arm.

Arguments

arm	A object of class Arm giving the arm.
-----	---------------------------------------

Value

A list giving the administration parameters of an arm.

BayesianFim

BayesianFim

Description

The class BayesianFim represents and stores information for the Bayesian Fim.

Usage

```
BayesianFim(
  fisherMatrix = numeric(0),
  fixedEffects = numeric(0),
  varianceEffects = numeric(0),
  SEAndRSE = list(),
  condNumberFixedEffects = 0,
  condNumberVarianceEffects = 0,
  shrinkage = numeric(0)
)
```

Arguments

fisherMatrix A matrix giving the numerical values of the Fim.

fixedEffects A matrix giving the numerical values of the fixedEffects of the Fim.

varianceEffects A matrix giving the numerical values of varianceEffects of the Fim.

SEAndRSE A data frame giving the value of the SE and RSE.

condNumberFixedEffects The conditional number of the fixedEffects of the Fim.

condNumberVarianceEffects The conditional number of the varianceEffects of the Fim.

shrinkage A vector giving the shrinkage values.

checkSamplingTimeConstraintsForMetaheuristic

checkSamplingTimeConstraintsForMetaheuristic

Description

checkSamplingTimeConstraintsForMetaheuristic

Arguments

samplingTimesConstraints	An object SamplingTimeConstraints.
arm	An object Arm.
newSamplings	A vector of numeric for the new samplings.
outcome	A string giving the outcome.

Value

A boolean TRUE/FALSE, with a message error if FALSE.

checkValiditySamplingConstraint	<i>checkValiditySamplingConstraint: check if the constraints used for the design optimization are valid.</i>
---------------------------------	--

Description

checkValiditySamplingConstraint: check if the constraints used for the design optimization are valid.

Arguments

design	An object Design giving the design.
--------	-------------------------------------

Value

A boolean TRUE / FALSE, if FALSE it also gives an error message.

Combined1	<i>Combined1</i>
-----------	------------------

Description

The class Combined1 represents and stores information for the error model Combined1.

Usage

```
Combined1(  
  output = character(0),  
  equation = expression(sigmaInter + sigmaSlope * output),  
  derivatives = list(),  
  sigmaInter = 0,  
  sigmaSlope = 0,  
  sigmaInterFixed = FALSE,  
  sigmaSlopeFixed = FALSE,  
  cError = 1  
)
```

Arguments

output	A string giving the model error output.
equation	A expression giving the model error equation.
derivatives	A list giving the derivatives of the model error equation.
sigmaInter	A double giving the sigma inter.
sigmaSlope	A double giving the sigma slope
sigmaInterFixed	A Boolean giving if the sigma inter is fixed or not. - not in the v7.0
sigmaSlopeFixed	A Boolean giving if the sigma slope is fixed or not. - not in the v7.0
cError	A integer giving the power parameter.

computeVMat	<i>computeVMat</i>
-------------	--------------------

Description

computeVMat

Usage

computeVMat(varParam1, varParam2, invCholV)

Arguments

varParam1	varParam1
varParam2	varParam2
invCholV	invCholV

Value

VMat

Constant	<i>Constant</i>
----------	-----------------

Description

The class Constant represents and stores information for the error model Constant.

Usage

```
Constant(  
    output = character(0),  
    equation = expression(sigmaInter),  
    derivatives = list(),  
    sigmaInter = 0,  
    sigmaSlope = 0,  
    sigmaInterFixed = FALSE,  
    sigmaSlopeFixed = FALSE,  
    cError = 1  
)
```

Arguments

- | | |
|-----------------|--|
| output | A string giving the model error output. |
| equation | A expression giving the model error equation. |
| derivatives | A list giving the derivatives of the model error equation. |
| sigmaInter | A double giving the sigma inter. |
| sigmaSlope | A double giving the sigma slope |
| sigmaInterFixed | A boolean giving if the sigma inter is fixed or not. |
| sigmaSlopeFixed | A boolean giving if the sigma slope is fixed or not. |
| cError | A integer giving the power parameter. |

constraintsTableForReport	<i>constraintsTableForReport: table of the PGBOAlgorithm constraints for the report.</i>
---------------------------	--

Description

- constraintsTableForReport: table of the PGBOAlgorithm constraints for the report.
- constraintsTableForReport: table of the PSOAlgorithm constraints for the report.
- constraintsTableForReport: table of the SimplexAlgorithm constraints for the report.
- constraintsTableForReport
- constraintsTableForReport: table of the MultiplicativeAlgorithm constraints for the report.

Arguments

- optimizationAlgorithm A object MultiplicativeAlgorithm.
- arms List of the arms.

Value

- The table for the constraints in the arms.
- The table for the constraints in the arms.
- The table for the constraints in the arms.
- armsConstraintsTable
- The table for the constraints in the arms.

convertPKModelAnalyticToPKModelODE	<i>convertPKModelAnalyticToPKModelODE: conversion from analytic to ode</i>
------------------------------------	--

Description

- convertPKModelAnalyticToPKModelODE: conversion from analytic to ode
- convertPKModelAnalyticToPKModelODE: conversion from analytic to ode
- convertPKModelAnalyticToPKModelODE: conversion from analytic infusion to ode

Arguments

- pkModel An object of class ModelAnalyticInfusion that defines the model.

Dcriterion	<i>Dcriterion: get the D-criterion of the Fim.</i>
------------	--

Description

- Dcriterion: get the D-criterion of the Fim.

Arguments

- Fim A object Fim giving the Fim.

Value

- A double giving the D-criterion of the Fim.

defineFim	<i>define the type of Fisher information matrix: population, individual or Bayesian</i>
-----------	---

Description

define the type of Fisher information matrix: population, individual or Bayesian

Arguments

pfimproject An object PFIMProject.

Value

An object Fim.

defineModelAdministration	<i>defineModelAdministration: define the administration</i>
---------------------------	---

Description

defineModelAdministration: define the administration
defineModelAdministration: define the administration
defineModelAdministration: define the administration
defineModelAdministration: define the administration
defineModelAdministration: define the administration
defineModelAdministration: define the administration
defineModelAdministration: define the administration

Arguments

model An object of class ModelODEInfusionDoseInEquation that defines the model.
arm An object of class Arm that defines the arm.

Value

The model with samplings, solverInputs
The model with samplings, solverInputs
The model with samplings, solverInputs
The model with updated slots.
The model with samplings, solverInputs
The model with samplings, solverInputs
The model with updated slots.

defineModelEquationsFromLibraryOfModel

defineModelEquationsFromLibraryOfModel: define the model equations giving the models in the library of models.

Description

defineModelEquationsFromLibraryOfModel: define the model equations giving the models in the library of models.

Arguments

pfimproject An object PFIMProject giving the evaluation to be run.

Value

A list giving the model equations.

defineModelType

defineModelType: define the class of the model to be evaluated.

Description

defineModelType: define the class of the model to be evaluated.

Arguments

pfimproject An object PFIMProject giving the evaluation to be run.

Value

An object Model giving the model to be evaluated with its modelParameters, odeSolverParameters, modelError, modelEquations.

defineModelWrapper	<i>defineModelWrapper: define the model wrapper for the ode solver</i>
--------------------	--

Description

defineModelWrapper: define the model wrapper for the ode solver
defineModelWrapper: define the model wrapper for the ode solver
defineModelWrapper: define the model wrapper for the ode solver
defineModelWrapper: define the model wrapper for the ode solver
defineModelWrapper: define the model wrapper for the ode solver
defineModelWrapper: define the model wrapper for the ode solver
defineModelWrapper: define the model wrapper for the ode solver
defineModelWrapper: define the model wrapper for the ode solver

Arguments

model	An object of class ModelODEInfusionDoseInEquation that defines the model.
evaluation	An object of class Evaluation that defines the evaluation

Value

The model with wrapperModelAnalytic, functionArgumentsModelAnalytic, functionArgumentsSymbolModelAnalytic, outputNames, outcomesWithAdministration

The model with wrapperModelAnalyticInfusion, functionArgumentsModelAnalyticInfusion, functionArgumentsSymbolModelAnalyticInfusion, outputNames, outcomesWithAdministration

The model with wrapperModelAnalyticInfusion, functionArgumentsModelAnalyticInfusion, functionArgumentsSymbolModelAnalyticInfusion, outputNames, outcomesWithAdministration

The model with wrapperModelAnalytic, functionArgumentsModelAnalytic, functionArgumentsSymbolModelAnalytic, outputNames, outcomesWithAdministration

The model with updated slots.

The model with the updated slots.

The model with the updated slots.

The model with updated slots.

defineOptimizationAlgorithm	<i>Define optimization algorithm</i>
-----------------------------	--------------------------------------

Description

Define optimization algorithm

Arguments

optimization An Optimization object.

Value

An optimization algorithm.

definePKModel	<i>definePKModel: define a PK model from library of model</i>
---------------	---

Description

definePKModel: define a PK model from library of model
definePKModel ModelAnalyticInfusion
definePKModel
definePKModel
definePKModel: define PK model ode bolus
definePKModel: define a PK model from library of model
definePKModel: define a PK model from library of model
definePKModel: define PK model ode bolus

Arguments

pkModel An object of class ModelODEInfusionDoseInEquation that defines the PK model.
pfimproject An object of class PFIMProject that defines the pfimproject.

definePKPDMModel	<i>definePKPDMModel: define a PKPD model from library of model</i>
------------------	--

Description

definePKPDMModel: define a PKPD model from library of model
definePKPDMModel: define a PKPD model from library of model
definePKPDMModel ModelAnalyticInfusion, ModelAnalytic
definePKPDMModel ModelAnalyticInfusion, ModelODE
definePKPDMModel
definePKPDMModel
definePKPDMModel
definePKPDMModel: define a PKPD model from library of model

Arguments

pkModel An object of class ModelODE that defines the PD model.
pfimproject An object of class PFIMProject that defines the pfimproject.

Design	<i>Design</i>
--------	---------------

Description

The class Design represents and stores information for the Design.

Usage

```
Design(  
  name = character(0),  
  size = 0,  
  arms = list(),  
  evaluationArms = list(),  
  numberOfArms = 0,  
  fim = Fim()  
)
```

Arguments

name A string giving the name of the design.
size A integer giving the size of the design.
arms A list giving the arms of the design.
evaluationArms A list giving the valuation of the arms of the design.
numberOfArms A integer giving the number of arms.
fim A object Fim giving the Fim of the design.

Details

Design

Distribution	<i>Distribution</i>
--------------	---------------------

Description

The class `Distribution` represents and stores information for the parameter distribution.

Usage

```
Distribution(name = character(0), mu = 0, omega = 0)
```

Arguments

- | | |
|-------|---|
| name | A string giving the name of the distribution. |
| mu | A double giving the mean μ . |
| omega | A double giving ω . |

<code>evaluateArm</code>	<i>evaluateArm: evaluation of the model with the arm parameters.</i>
--------------------------	--

Description

`evaluateArm`: evaluation of the model with the arm parameters.

Arguments

- | | |
|-------|--|
| arm | A object of class <code>Arm</code> giving the arm. |
| model | A object of class <code>Model</code> giving the model. |
| fim | A object of class <code>Fim</code> giving the fim. |

Value

The object arm with the slots `evaluationModel`, `evaluationGradients`, `evaluationVariance` and `evaluationFim`.

evaluateDesign	<i>evaluateDesign: evaluation of a design.</i>
----------------	--

Description

evaluateDesign: evaluation of a design.

Arguments

design	An object Design giving the design.
model	An object Model giving the model.
fim	An object Fim giving the Fim.

Value

The object Design with its evaluation results.

evaluateErrorModelDerivatives	<i>evaluateErrorModelDerivatives; evaluate the derivatives of the model error.</i>
-------------------------------	--

Description

evaluateErrorModelDerivatives; evaluate the derivatives of the model error.

Arguments

modelError	An object ModelError that defines the model error.
evaluationModel	A dataframe giving the outputs for the model evaluation.

Value

The matrices sigmaDerivatives and errorVariance.

evaluateFim	<i>evaluateFim: evaluation of the Fim</i>
-------------	---

Description

evaluateFim: evaluation of the Fim

evaluateFim: evaluation of the Fim

evaluateFim: evaluation of the Fim

Arguments

fim	An object PopulationFim giving the Fim.
model	An object Model giving the model.
arm	An object Arm giving the arm.

Value

The object Fim with the fisherMatrix and the shrinkage.

The object IndividualFim with the fisherMatrix and the shrinkage.

The object IndividualFim with the fisherMatrix and the shrinkage.

evaluateInitialConditions	<i>evaluateInitialConditions: evaluate the initial conditions.</i>
---------------------------	--

Description

evaluateInitialConditions: evaluate the initial conditions.

evaluateInitialConditions: evaluate the initial conditions.

evaluateInitialConditions: evaluate the initial conditions.

Arguments

arm	A object of class Arm giving the arm.
model	A object of class ModelODEInfusion giving the model.
doseEvent	A data frame giving the dose event for the ode solver.

Value

A list giving the evaluated initial conditions.

evaluateModel	<i>evaluateModel: evaluate the model</i>
---------------	--

Description

evaluateModel: evaluate the model
evaluateModel: evaluate the ModelAnalyticInfusion
evaluateModel: evaluate the ModelAnalyticInfusion
evaluateModel: evaluate the ModelAnalyticInfusion
evaluateModel
evaluateModel
evaluateModel: evaluate the model
evaluateModel: evaluate the model
evaluateModel

Arguments

arm A object of class Arm giving the arm.
model A object of class ModelODEInfusionDoseInEquation giving the model.

Value

A list of dataframes that contains the results for the evaluation of the model.
A list of dataframes that contains the results for the evaluation of the model.
A list of dataframes that contains the results for the evaluation of the model.
A list of dataframes that contains the results for the evaluation of the model.
A list of dataframes that contains the evaluation of the model.
A data frame giving the output of the model evaluation.
A list of dataframes that contains the results for the evaluation of the model.
A list of dataframes that contains the results for the evaluation of the model.
A data frame giving the output of the model evaluation.

evaluateModelGradient	<i>evaluateModelGradient: evaluate the gradient of the model</i>
-----------------------	--

Description

evaluateModelGradient: evaluate the gradient of the model

Arguments

model	An object Model that defines the model.
arm	A object Arm giving the arm

Value

A data frame that contains the gradient of the model.

evaluateModelVariance	<i>evaluateModelVariance: evaluate the variance of the model</i>
-----------------------	--

Description

evaluateModelVariance: evaluate the variance of the model

Arguments

model	A object Model giving the model.
arm	A object Arm giving the arm

Value

A list giving errorVariance and sigmaDerivatives.

evaluateVarianceFIM	<i>evaluateVarianceFIM: evaluate the variance</i>
---------------------	---

Description

evaluateVarianceFIM: evaluate the variance
evaluateVarianceFIM: evaluate the variance
evaluateVarianceFIM: evaluate the variance

Arguments

arm A object of class Arm giving the arm.
model A object of class Model giving the model.
fim A object of class PopulationFim giving the Fim.

Value

The matrices MFbeta and V.
The matrices MFbeta and V.
The matrices MFVar and V.

Evaluation	<i>Evaluation</i>
------------	-------------------

Description

The class Evaluation represents and stores information for the evaluation of a design

Usage

```
Evaluation(  
  evaluationDesign = list(),  
  name = character(0),  
  modelParameters = list(),  
  modelEquations = list(),  
  modelFromLibrary = list(),  
  modelError = list(),  
  designs = list(),  
  outputs = list(),  
  fimType = character(0),  
  odeSolverParameters = list()  
)
```

Arguments

evaluationDesign	A list giving the evaluation of the design.
name	A string giving the name of the design evaluation.
modelParameters	A list giving the model parameters.
modelEquations	A list giving the model equations.
modelFromLibrary	A list giving the model equations from the library of model.
modelError	A list giving the model error.
designs	A list giving the designs to be evaluated.
outputs	A list giving the model outputs.
fimType	A string giving the type of Fim being evaluated.
odeSolverParameters	A list giving the atol and rtol parameters for the ode solver.

FedorovWynnAlgorithm *FedorovWynnAlgorithm*

Description

The class FedorovWynnAlgorithm implements the FedorovWynn algorithm.

Usage

```
FedorovWynnAlgorithm(
  name = character(0),
  modelEquations = list(),
  modelFromLibrary = list(),
  modelParameters = list(),
  modelError = list(),
  optimizer = character(0),
  optimizerParameters = list(),
  outputs = list(),
  designs = list(),
  fimType = character(0),
  fim = Fim(),
  odeSolverParameters = list(),
  optimisationDesign = list(),
  optimisationAlgorithmOutputs = list(),
  elementaryProtocols = list(),
  numberOfSubjects = 0,
  proportionsOfSubjects = 0,
  showProcess = FALSE,
  FedorovWynnAlgorithmOutputs = list()
)
```

Arguments

name	A string giving the name of the design evaluation.
modelEquations	A list giving the model equations.
modelFromLibrary	A list giving the model equations from the library of model.
modelParameters	A list giving the model parameters.
modelError	A list giving the model error.
optimizer	A string giving the name of the optimization algorithm being used.
optimizerParameters	A list giving the parameters of the optimization algorithm.
outputs	A list giving the model outputs.
designs	A list giving the designs to be evaluated.
fimType	A string giving the type of Fim being evaluated.
fim	A object Fim giving the Fim.
odeSolverParameters	A list giving the atol and rtol parameters for the ode solver.
optimisationDesign	A list giving the evaluation of initial and optimal design.
optimisationAlgorithmOutputs	A list giving the outputs of the optimization process.
elementaryProtocols	List of elementary protocols
numberOfSubjects	Numeric vector specifying number of subjects
proportionsOfSubjects	Numeric vector of subject proportions
showProcess	Logical indicating whether to show process
FedorovWynnAlgorithmOutputs	A list giving the output of the optimization algorithm.

FedorovWynnAlgorithm_Rcpp

Fedorov-Wynn algorithm in Rcpp.

Description

Run the FedorovWynnAlgorithm in Rcpp

Usage

```
FedorovWynnAlgorithm_Rcpp(  
  protocols_input,  
  ndimen_input,  
  nbprot_input,  
  numprot_input,  
  freq_input,  
  nbdata_input,  
  vectps_input,  
  fisher_input,  
  nok_input,  
  protdep_input,  
  freqdep_input  
)
```

Arguments

protocols_input	parameter protocols_input
ndimen_input	parameter ndimen_input
nbprot_input	parameter nbprot_input
numprot_input	parameter numprot_input
freq_input	parameter freq_input
nbdata_input	parameter nbdata_input
vectps_input	parameter vectps_input
fisher_input	parameter fisher_input
nok_input	parameter nok_input
protdep_input	parameter protdep_input
freqdep_input	parameter freqdep_input

Value

A list giving the results of the outputs of the FedorovWynn algorithm.

Fim	<i>Fim</i>
-----	------------

Description

The class Fim represents and stores information for the Fim.

Usage

```
Fim(
  fisherMatrix = numeric(0),
  fixedEffects = numeric(0),
  varianceEffects = numeric(0),
  SEAndRSE = list(),
  condNumberFixedEffects = 0,
  condNumberVarianceEffects = 0,
  shrinkage = numeric(0)
)
```

Arguments

fisherMatrix	A matrix giving the numerical values of the Fim.
fixedEffects	A matrix giving the numerical values of the fixedEffects of the Fim.
varianceEffects	A matrix giving the numerical values of varianceEffects of the Fim.
SEAndRSE	A data frame giving the value of the SE and RSE.
condNumberFixedEffects	The conditional number of the fixedEffects of the Fim.
condNumberVarianceEffects	The conditional number of the varianceEffects of the Fim.
shrinkage	A vector giving the shrinkage values.

finiteDifferenceHessian

finiteDifferenceHessian: compute the Hessian

Description

finiteDifferenceHessian: compute the Hessian

Arguments

model	A object Model giving the model.
-------	----------------------------------

Value

The model with the slots parametersForComputingGradient with XcolsInv, shifted, frac.

fisherSimplex	<i>Compute the fisher.simplex</i>
---------------	-----------------------------------

Description

Compute the fisher.simplex

Arguments

simplex	A list giving the parameters of the simplex.
optimizationObject	An object Optimization.
outcomes	A vector giving the outcomes of the arms.

Value

A list giving the results of the optimization.

fun.amoeba	<i>Compute the fun.amoeba</i>
------------	-------------------------------

Description

Compute the fun.amoeba

Usage

```
fun.amoeba(p, y, ftol, itmax, funk, outcomes, data, showProcess)
```

Arguments

p	parameter p
y	parameter y
ftol	parameter ftol
itmax	parameter itmax
funk	parameter funk
outcomes	The model outcomes.
data	parameter data
showProcess	Boolean.

Value

fun.amoeba

`generateDosesCombination`*generateDosesCombination: generate the combination for the doses.*

Description

generateDosesCombination: generate the combination for the doses.

Arguments

design An object Design giving the design.

Value

dosesForFIMs, numberOfDoses used in the design optimization.

`generateFimsFromConstraints`*Generate FIMs from constraints*

Description

Generate FIMs from constraints

Arguments

optimization An Optimization object.

Value

A list containing FIMs from constraints.

Arguments

fim An object PopulationFim giving the Fim.
 optimizationAlgorithm An object PGBOAlgorithm giving the PGBOAlgorithm
 tablesForReport The output list giving by the method tablesForReport.

Value

The html report for the design optimization.
 The html report for the design optimization.
 The html report.
 The html report.
 The html report.
 The html report.
 The html report.
 The html report.
 The html report.
 The html report.
 The html report.
 The html report.

generateSamplingsFromSamplingConstraints
generateSamplingsFromSamplingConstraints

Description

generateSamplingsFromSamplingConstraints

Arguments

samplingTimeConstraints An object SamplingTimeConstraints

Value

A list intervalsConstraints.

generateSamplingTimesCombination

generateSamplingTimesCombination: generate the combination for the samplings.

Description

generateSamplingTimesCombination: generate the combination for the samplings.

Arguments

design An object Design giving the design.

Value

samplingTimesCombinations used in the design optimization.

getArmConstraints

getArmConstraints: get the administration and sampling time constraints for the MultiplicativeAlgorithm.

Description

getArmConstraints: get the administration and sampling time constraints for the MultiplicativeAlgorithm.

getArmConstraints: get the administration and sampling time constraints for the FedorovWynnAlgorithm.

getArmConstraints: get the administration and sampling time constraints for the SimplexAlgorithm.

getArmConstraints: get the administration and sampling time constraints for the PSOAlgorithm.

getArmConstraints: get the administration and sampling time constraints for the PGBOAlgorithm.

Arguments

arm A object of class Arm giving the arm.

optimizationAlgorithm A object of class Optimization giving the optimization algorithm.

Value

A list giving the administration and sampling time constraints for the MultiplicativeAlgorithm.

A list giving the administration and sampling time constraints for the FedorovWynnAlgorithm.

A list giving the administration and sampling time constraints for the SimplexAlgorithm.

A list giving the administration and sampling time constraints for the PSOAlgorithm.

A list giving the administration and sampling time constraints for the PGBOAlgorithm.

getArmData	<i>getArmData: extract arm data for The Report</i>
------------	--

Description

getArmData: extract arm data for The Report

Arguments

arm	A object of class Arm giving the arm.
-----	---------------------------------------

Value

A list giving the name, Number of subjects, Outcome, Dose and Sampling times of the arm.

getCorrelationMatrix	<i>getCorrelationMatrix : get the correlation matrix</i>
----------------------	--

Description

getCorrelationMatrix : get the correlation matrix

getCorrelationMatrix : get the correlation matrix

Arguments

pfimproject	A object PFIMProject giving the Evaluation.
-------------	---

Value

The correlation matrix

The Dcriterion

getDcriterion	<i>getDcriterion : get the Dcriterion</i>
---------------	---

Description

getDcriterion : get the Dcriterion
getDcriterion : get the Dcriterion

Arguments

pfimproject A object PFIMProject giving the Evaluation.

Value

The Dcriterion of the FIM.
The Dcriterion

getDeterminant	<i>getDeterminant: get the determinant</i>
----------------	--

Description

getDeterminant: get the determinant
getDeterminant: get the determinant

Arguments

pfimproject A object PFIMProject giving the Evaluation.

Value

The determinant of the FIM.
The determinant

getFim	<i>getFim: get the Fisher matrix.</i>
--------	---------------------------------------

Description

getFim: get the Fisher matrix.

Arguments

evaluation An object Evaluation giving the evaluation to be run.

Value

The matrices fisherMatrix, fixedEffects, varianceEffects.

getFisherMatrix	<i>getFisherMatrix: display the Fisher matrix components</i>
-----------------	--

Description

getFisherMatrix: display the Fisher matrix components

getFisherMatrix: display the Fisher matrix components

Arguments

evaluation An object Evaluation giving the evaluation to be run.

Value

The matrices fisherMatrix, fixedEffects, varianceEffects.

The matrices fisherMatrix, fixedEffects, varianceEffects.

getListLastName	<i>getListLastName: routine to get the names of last element of a nested list.</i>
-----------------	--

Description

getListLastName: routine to get the names of last element of a nested list.

Usage

```
getListLastName(list)
```

Arguments

list	The list to be used.
------	----------------------

Value

The names of last element.

getModelErrorData	<i>getModelErrorData: get the parameters sigma slope and sigma inter (used for the report).</i>
-------------------	---

Description

getModelErrorData: get the parameters sigma slope and sigma inter (used for the report).

Arguments

modelError	An object ModelError that defines the model error.
------------	--

Value

A list of dataframe with outcome, type of model error and sigma slope and inter.

`getModelParametersData`*getModelParametersData: get model parameters data for report.*

Description

`getModelParametersData`: get model parameters data for report.

Arguments

`modelParameter` An object if class `Model` giving the model.

Value

A data frame with the data of all the parameters.

`getRSE`*getRSE: get the RSE*

Description

`getRSE`: get the RSE

`getRSE`: get the RSE

Arguments

`pfimproject` A object `PFIMProject` giving the Evaluation.

Value

The RSE of the parameters.

The RSE

getSamplingData	<i>getSamplingData: extract sampling times and max sampling time used for plot.</i>
-----------------	---

Description

getSamplingData: extract sampling times and max sampling time used for plot.

Arguments

arm A object of class Arm giving the arm.

Value

A list giving the samplingTimes object, the vector samplings and the double samplingMax.

getSE	<i>getSE: get the SE</i>
-------	--------------------------

Description

getSE: get the SE

getSE: get the SE

Arguments

pfimproject A object PFIMProject giving the Evaluation.

Value

The SE of the parameters.

The SE.

getShrinkage	<i>getShrinkage: get the shrinkage</i>
--------------	--

Description

getShrinkage: get the shrinkage
getShrinkage: get the shrinkage

Arguments

pfimproject A object PFIMProject giving the Evaluation.

Value

The shrinkage of the FIM.
The shrinkage

IndividualFim	<i>IndividualFim</i>
---------------	----------------------

Description

The class IndividualFim represents and stores information for the IndividualFim.

Usage

```
IndividualFim(  
  fisherMatrix = numeric(0),  
  fixedEffects = numeric(0),  
  varianceEffects = numeric(0),  
  SEAndRSE = list(),  
  condNumberFixedEffects = 0,  
  condNumberVarianceEffects = 0,  
  shrinkage = numeric(0)  
)
```

Arguments

fisherMatrix A matrix giving the numerical values of the Fim.
fixedEffects A matrix giving the numerical values of the fixedEffects of the Fim.
varianceEffects A matrix giving the numerical values of varianceEffects of the Fim.
SEAndRSE A data frame giving the value of the SE and RSE.

condNumberFixedEffects

The conditional number of the fixedEffects of the Fim.

condNumberVarianceEffects

The conditional number of the varianceEffects of the Fim.

shrinkage

A vector giving the shrinkage values.

LibraryOfModels

LibraryOfModels

Description

The class LibraryOfModels represents and stores information for the LibraryOfModels.

Usage

```
LibraryOfModels(models = list())
```

Arguments

models

A list giving all the PK and PD models.

LibraryOfPDModels

LibraryOfPDModels

Description

The class LibraryOfPDModels represents and stores information for the LibraryOfPDModels.

Usage

```
LibraryOfPDModels
```

Format

An object of class PFIM::LibraryOfPDModels (inherits from PFIM::LibraryOfModels, S7_object) of length 1.

LibraryOfPKModels	<i>LibraryOfPKModels</i>
-------------------	--------------------------

Description

The class LibraryOfPKModels represents and stores information for the LibraryOfPKModels.

Usage

LibraryOfPKModels

Format

An object of class PFIM::LibraryOfPKModels (inherits from PFIM::LibraryOfModels, S7_object) of length 1.

Linear2BolusSingleDose_C1QV1V2	<i>Model Linear2BolusSingleDose_C1QV1V2</i>
--------------------------------	---

Description

Model Linear2BolusSingleDose_C1QV1V2

Usage

Linear2BolusSingleDose_C1QV1V2()

Linear2BolusSingleDose_kk12k21V	<i>Model Linear2BolusSingleDose_kk12k21V</i>
---------------------------------	--

Description

Model Linear2BolusSingleDose_kk12k21V

Usage

Linear2BolusSingleDose_kk12k21V()

Linear2BolusSteadyState_ClQV1V2tau

Model Linear2BolusSteadyState_ClQV1V2tau

Description

Model Linear2BolusSteadyState_ClQV1V2tau

Usage

Linear2BolusSteadyState_ClQV1V2tau()

Linear2BolusSteadyState_kk12k21Vtau

Model Linear2BolusSteadyState_kk12k21Vtau

Description

Model Linear2BolusSteadyState_kk12k21Vtau

Usage

Linear2BolusSteadyState_kk12k21Vtau()

Linear2FirstOrderSingleDose_kaClQV1V2

Model Linear2FirstOrderSingleDose_kaClQV1V2

Description

Model Linear2FirstOrderSingleDose_kaClQV1V2

Usage

Linear2FirstOrderSingleDose_kaClQV1V2()

Linear2FirstOrderSingleDose_kakk12k21V

Model Linear2FirstOrderSingleDose_kakk12k21V

Description

Model Linear2FirstOrderSingleDose_kakk12k21V

Usage

Linear2FirstOrderSingleDose_kakk12k21V()

Linear2FirstOrderSteadyState_kaClQV1V2tau

Model Linear2FirstOrderSteadyState_kaClQV1V2tau

Description

Model Linear2FirstOrderSteadyState_kaClQV1V2tau

Usage

Linear2FirstOrderSteadyState_kaClQV1V2tau()

Linear2FirstOrderSteadyState_kakk12k21Vtau

Model Linear2FirstOrderSteadyState_kakk12k21Vtau

Description

Model Linear2FirstOrderSteadyState_kakk12k21Vtau

Usage

Linear2FirstOrderSteadyState_kakk12k21Vtau()

Linear2InfusionSingleDose_ClQV1V2
<i>Model Linear2InfusionSingleDose_ClQV1V2</i>

Description

Model Linear2InfusionSingleDose_ClQV1V2

Usage

Linear2InfusionSingleDose_ClQV1V2()

Linear2InfusionSingleDose_kk12k21V
<i>Model Linear2InfusionSingleDose_kk12k21V</i>

Description

Model Linear2InfusionSingleDose_kk12k21V

Usage

Linear2InfusionSingleDose_kk12k21V()

Linear2InfusionSteadyState_ClQV1V2tau
<i>Model Linear2InfusionSteadyState_ClQV1V2tau</i>

Description

Model Linear2InfusionSteadyState_ClQV1V2tau

Usage

Linear2InfusionSteadyState_ClQV1V2tau()

Linear2InfusionSteadyState_kk12k21Vtau
<i>Model Linear2InfusionSteadyState_kk12k21Vtau</i>

Description

Model Linear2InfusionSteadyState_kk12k21Vtau

Usage

Linear2InfusionSteadyState_kk12k21Vtau()

LogNormal	<i>LogNormal</i>
-----------	------------------

Description

The class LogNormal implements the LogNormal distribution.

Usage

LogNormal(name = character(0), mu = 0, omega = 0)

Arguments

- | | |
|-------|---|
| name | A string giving the name of the distribution. |
| mu | A double giving the mean mu. |
| omega | A double giving omega. |

Model	<i>Model</i>
-------	--------------

Description

The class Model represents and stores information for a model.

Usage

```

Model(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list()
)

```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols

ModelAnalytic

ModelAnalytic

Description

The class ModelAnalytic is used to defined an analytic model.

Usage

```
ModelAnalytic(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list(),
  wrapperModelAnalytic = list(),
  functionArgumentsModelAnalytic = list(),
  functionArgumentsSymbolModelAnalytic = list(),
  solverInputs = list()
)
```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration

outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols
wrapperModelAnalytic	Wrapper for the ode solver.
functionArgumentsModelAnalytic	A list giving the functionArguments of the wrapper for the analytic model.
functionArgumentsSymbolModelAnalytic	A list giving the functionArgumentsSymbol of the wrapper for the analytic model
solverInputs	A list giving the solver inputs.

ModelAnalyticInfusion *ModelAnalyticInfusion*

Description

The class ModelAnalyticInfusion is used to defined an analytic model in infusion.

Usage

```
ModelAnalyticInfusion(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
```

```

initialConditions = numeric(0),
functionArguments = character(0),
functionArgumentsSymbol = list(),
wrapperModelAnalyticInfusion = list(),
functionArgumentsModelAnalyticInfusion = list(),
functionArgumentsSymbolModelAnalyticInfusion = list(),
solverInputs = list()
)

```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols
wrapperModelAnalyticInfusion	Wrapper for the ode solver.
functionArgumentsModelAnalyticInfusion	A list giving the functionArguments of the wrapper for the analytic model in infusion.
functionArgumentsSymbolModelAnalyticInfusion	A list giving the functionArgumentsSymbol of the wrapper for the analytic model in infusion.
solverInputs	A list giving the solver inputs.

ModelAnalyticInfusionSteadyState

ModelAnalyticInfusionSteadyState

Description

The class ModelAnalyticInfusionSteadyState is used to defined an analytic model in infusion steady state.

Usage

```
ModelAnalyticInfusionSteadyState(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list(),
  wrapperModelAnalyticInfusion = list(),
  functionArgumentsModelAnalyticInfusion = list(),
  functionArgumentsSymbolModelAnalyticInfusion = list(),
  solverInputs = list()
)
```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names

outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols
wrapperModelAnalyticInfusion	Wrapper for the ode solver.
functionArgumentsModelAnalyticInfusion	A list giving the functionArguments of the wrapper for the analytic model in infusion.
functionArgumentsSymbolModelAnalyticInfusion	A list giving the functionArgumentsSymbol of the wrapper for the analytic model in infusion.
solverInputs	A list giving the solver inputs.

Details

ModelAnalyticInfusionSteadyState

ModelAnalyticSteadyState

ModelAnalyticSteadyState

Description

The class ModelAnalyticSteadyState is used to defined an analytic model in steady state.

Usage

```
ModelAnalyticSteadyState(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
```

```

outputFormula = list(),
outputNames = character(0),
variableNames = character(0),
outcomesWithAdministration = character(0),
outcomesWithNoAdministration = character(0),
modelError = list(),
odeSolverParameters = list(),
parametersForComputingGradient = list(),
initialConditions = numeric(0),
functionArguments = character(0),
functionArgumentsSymbol = list(),
wrapperModelAnalytic = list(),
functionArgumentsModelAnalytic = list(),
functionArgumentsSymbolModelAnalytic = list(),
solverInputs = list()
)

```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols
wrapperModelAnalytic	Wrapper for the ode solver.

functionArgumentsModelAnalytic	A list giving the functionArguments of the wrapper for the analytic model in steady state.
functionArgumentsSymbolModelAnalytic	A list giving the functionArgumentsSymbol of the wrapper for the analytic model in steady state.
solverInputs	A list giving the solver inputs.

Details

ModelAnalyticSteadyState

ModelError	<i>ModelError</i>
------------	-------------------

Description

The class ModelError is used to defined a model error.

Usage

```
ModelError(  
  output = "output",  
  equation = expression(),  
  derivatives = list(),  
  sigmaInter = 0.1,  
  sigmaSlope = 0,  
  sigmaInterFixed = FALSE,  
  sigmaSlopeFixed = FALSE,  
  cError = 1  
)
```

Arguments

output	A string giving the model error output.
equation	A expression giving the model error equation.
derivatives	A list giving the derivatives of the model error equation.
sigmaInter	A double giving the sigma inter.
sigmaSlope	A double giving the sigma slope
sigmaInterFixed	A boolean giving if the sigma inter is fixed or not. - not in the v7.0
sigmaSlopeFixed	A boolean giving if the sigma slope is fixed or not. - not in the v7.0
cError	A integer giving the power parameter.

Details

ModelError

ModelInfusion

ModelInfusion

Description

The class ModelInfusion is used to defined a model in infusion.

Usage

```
ModelInfusion(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list()
)
```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model

odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols

ModelODE

ModelODE

Description

The class ModelODE is used to defined a ode model.

Usage

```
ModelODE(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list()
)
```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations

wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols

ModelODEBolus

ModelODEBolus

Description

The class ModelODEBolus is used to defined a model ode admin bolus.

Usage

```
ModelODEBolus(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
```

```

functionArgumentsSymbol = list(),
modelODE = function() NULL,
doseEvent = list(),
solverInputs = list()
)

```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols
modelODE	An object modelODE.
doseEvent	A dataframe given the doseEvent for the ode solver.
solverInputs	A list giving the solver inputs.

ModelODEDoseInEquations

ModelODEDoseNotInEquations

Description

The class ModelODEDoseNotInEquations is used to defined a ModelODEDoseNotInEquations

Usage

```
ModelODEDoseInEquations(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list(),
  modelODEDoseInEquations = function() NULL,
  solverInputs = list()
)
```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration

outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols
modelODEDoseInEquations	An object modelODEDoseInEquations.
solverInputs	A list giving the solver inputs.

ModelODEDoseNotInEquations

ModelODEDoseNotInEquations

Description

The class ModelODEDoseNotInEquations is used to defined a ModelODEDoseNotInEquations

Usage

```
ModelODEDoseNotInEquations(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list(),
  modelODE = function() NULL,
  doseEvent = list(),
  solverInputs = list()
)
```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols
modelODE	An object modelODE.
doseEvent	A dataframe given the doseEvent for the ode solver.
solverInputs	A list giving the solver inputs.

ModelODEInfusion

ModelODEInfusion

Description

The class ModelODEInfusion is used to defined a model ModelODEInfusion.

Usage

```

ModelODEInfusion(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list()
)

```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names
outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols

ModelODEInfusionDoseInEquation

ModelODEInfusionDoseInEquation

Description

The class ModelODEInfusionDoseInEquation is used to defined a ModelODEInfusionDoseInEquation

Usage

```
ModelODEInfusionDoseInEquation(
  name = character(0),
  modelParameters = list(),
  samplings = numeric(0),
  modelEquations = list(),
  wrapper = function() NULL,
  outputFormula = list(),
  outputNames = character(0),
  variableNames = character(0),
  outcomesWithAdministration = character(0),
  outcomesWithNoAdministration = character(0),
  modelError = list(),
  odeSolverParameters = list(),
  parametersForComputingGradient = list(),
  initialConditions = numeric(0),
  functionArguments = character(0),
  functionArgumentsSymbol = list(),
  modelODE = function() NULL,
  wrapperModelInfusion = list(),
  solverInputs = list()
)
```

Arguments

name	Character vector specifying the model name
modelParameters	List of model parameters
samplings	Numeric vector of sampling times
modelEquations	List containing the model equations
wrapper	Function wrapper for the model (default: function () NULL)
outputFormula	List of output formulas
outputNames	Character vector of output names
variableNames	Character vector of variable names

outcomesWithAdministration	Character vector of outcomes with administration
outcomesWithNoAdministration	Character vector of outcomes without administration
modelError	List defining the error model
odeSolverParameters	List of ODE solver parameters
parametersForComputingGradient	List of parameters for gradient computation
initialConditions	Numeric vector of initial conditions
functionArguments	Character vector of function arguments
functionArgumentsSymbol	List of function argument symbols
modelODE	An object modelODE.
wrapperModelInfusion	Wrapper for solver.
solverInputs	A list giving the solver inputs.

ModelParameter

ModelParameter

Description

The class ModelParameter is used to defined the model parameters.

Usage

```
ModelParameter(
  name = character(0),
  distribution = Distribution(),
  fixedMu = FALSE,
  fixedOmega = FALSE
)
```

Arguments

name	A string giving the name of the parameter.
distribution	A string giving the distribution of the parameter.
fixedMu	A Boolean setting TRUE/FALSE if the mu is estimated or not.
fixedOmega	A Boolean setting TRUE/FALSE if the omega is estimated or not.

Details

ModelParameter

MultiplicativeAlgorithm

MultiplicativeAlgorithm

Description

The class MultiplicativeAlgorithm implements the multiplicative algorithm.

Usage

```
MultiplicativeAlgorithm(
    name = character(0),
    modelEquations = list(),
    modelFromLibrary = list(),
    modelParameters = list(),
    modelError = list(),
    optimizer = character(0),
    optimizerParameters = list(),
    outputs = list(),
    designs = list(),
    fimType = character(0),
    fim = Fim(),
    odeSolverParameters = list(),
    optimisationDesign = list(),
    optimisationAlgorithmOutputs = list(),
    lambda = 0,
    delta = 0,
    numberOfIterations = 0,
    weightThreshold = 0,
    showProcess = FALSE,
    multiplicativeAlgorithmOutputs = list()
)
```

Arguments

name	A string giving the name of the design evaluation.
modelEquations	A list giving the model equations.
modelFromLibrary	A list giving the model equations from the library of model.
modelParameters	A list giving the model parameters.
modelError	A list giving the model error.
optimizer	A string giving the name of the optimization algorithm being used.
optimizerParameters	A list giving the parameters of the optimization algorithm.

outputs	A list giving the model outputs.
designs	A list giving the designs to be evaluated.
fimType	A string giving the type of Fim being evaluated.
fim	A object Fim giving the Fim.
odeSolverParameters	A list giving the atol and rtol parameters for the ode solver.
optimisationDesign	A list giving the evaluation of initial and optimal design.
optimisationAlgorithmOutputs	A list giving the outputs of the optimization process.
lambda	A numeric giving the parameter lambda.
delta	A numeric giving the parameter delta
numberOfIterations	A numeric giving the number of iterations.
weightThreshold	A numeric giving the weight threshold.
showProcess	A Boolean for displaying the process or not.
multiplicativeAlgorithmOutputs	A list giving the output of the optimization algorithm.

MultiplicativeAlgorithm_Rcpp

Function MultiplicativeAlgorithm_Rcpp

Description

Run the MultiplicativeAlgorithm_Rcpp in Rcpp.

Usage

```
MultiplicativeAlgorithm_Rcpp(
  fisherMatrices_input,
  numberOfFisherMatrices_input,
  weights_input,
  numberOfParameters_input,
  dim_input,
  lambda_input,
  delta_input,
  iterationInit_input
)
```

Arguments

- fisherMatrices_input The parameter fotfisherMatrices_input.
- numberOfFisherMatrices_input The parameter numberOfFisherMatrices_input.
- weights_input The parameter weights_input.
- numberOfParameters_input The parameter numberOfParameters_input.
- dim_input The parameter dim_input.
- lambda_input The parameter lambda_input.
- delta_input The parameter delta_input.
- iterationInit_input The parameter iterationInit_input.

Value

The list output with the outputs of the MultiplicativeAlgorithm_Rcpp.

Normal	<i>Normal</i>
--------	---------------

Description

The class Normal implements the Normal distribution.

Usage

Normal(name = character(0), mu = 0, omega = 0)

Arguments

- name A string giving the name of the distribution.
- mu A double giving the mean mu.
- omega A double giving omega.

Optimization

Optimization

Description

The class Optimization implements the Optimization.

Usage

```
Optimization(
    name = character(0),
    modelEquations = list(),
    modelFromLibrary = list(),
    modelParameters = list(),
    modelError = list(),
    optimizer = character(0),
    optimizerParameters = list(),
    outputs = list(),
    designs = list(),
    fimType = character(0),
    fim = Fim(),
    odeSolverParameters = list(),
    optimisationDesign = list(),
    optimisationAlgorithmOutputs = list()
)
```

Arguments

name	A string giving the name of the design evaluation.
modelEquations	A list giving the model equations.
modelFromLibrary	A list giving the model equations from the library of model.
modelParameters	A list giving the model parameters.
modelError	A list giving the model error.
optimizer	A string giving the name of the optimization algorithm being used.
optimizerParameters	A list giving the parameters of the optimization algorithm.
outputs	A list giving the model outputs.
designs	A list giving the designs to be evaluated.
fimType	A string giving the type of Fim being evaluated.
fim	A object Fim giving the Fim.
odeSolverParameters	A list giving the atol and rtol parameters for the ode solver.

- optimisationDesign
 - A list giving the evaluation of initial and optimal design.
- optimisationAlgorithmOutputs
 - A list giving the outputs of the optimization process.

optimizedDesign	<i>Optimization PGBOAlgorithm</i>
-----------------	-----------------------------------

Description

- Optimization PGBOAlgorithm
- Optimization PSOAlgorithm
- Optimization SimplexAlgorithm
- Optimization FedorovWynnAlgorithm
- Optimization MultiplicativeAlgorithm

Arguments

- optimizationObject
 - A object Optimization.
- optimizationAlgorithm
 - A object MultiplicativeAlgorithm.

Value

- The object optimizationObject with the slots updated.
- The object optimizationObject with the slots updated.
- The object optimizationObject with the slots updated.
- The object optimizationObject with the slots updated.
- The object optimizationObject with the slots updated.

PFIMProject	<i>PFIMProject</i>
-------------	--------------------

Description

- The class PFIMProject implements the PFIM project.

Usage

```

PFIMProject(
    name = character(0),
    modelEquations = list(),
    modelFromLibrary = list(),
    modelParameters = list(),
    modelError = list(),
    optimizer = character(0),
    optimizerParameters = list(),
    outputs = list(),
    designs = list(),
    fimType = character(0),
    fim = Fim(),
    odeSolverParameters = list()
)

```

Arguments

name	A string giving the name of the design evaluation.
modelEquations	A list giving the model equations.
modelFromLibrary	A list giving the model equations from the library of model.
modelParameters	A list giving the model parameters.
modelError	A list giving the model error.
optimizer	A string giving the name of the optimization algorithm being used.
optimizerParameters	A list giving the parameters of the optimization algorithm.
outputs	A list giving the model outputs.
designs	A list giving the designs to be evaluated.
fimType	A string giving the type of Fim being evaluated.
fim	A object Fim giving the Fim.
odeSolverParameters	A list giving the atol and rtol parameters for the ode solver.

PGBOAlgorithm

PGBOAlgorithm

Description

The class PGBOAlgorithm implements the PGBO algorithm.

Usage

```

PGBOAlgorithm(
  name = character(0),
  modelEquations = list(),
  modelFromLibrary = list(),
  modelParameters = list(),
  modelError = list(),
  optimizer = character(0),
  optimizerParameters = list(),
  outputs = list(),
  designs = list(),
  fimType = character(0),
  fim = Fim(),
  odeSolverParameters = list(),
  optimisationDesign = list(),
  optimisationAlgorithmOutputs = list(),
  N = numeric(0),
  muteEffect = numeric(0),
  maxIteration = numeric(0),
  purgeIteration = numeric(0),
  seed = numeric(0),
  showProcess = FALSE
)

```

Arguments

<code>name</code>	A string giving the name of the design evaluation.
<code>modelEquations</code>	A list giving the model equations.
<code>modelFromLibrary</code>	A list giving the model equations from the library of model.
<code>modelParameters</code>	A list giving the model parameters.
<code>modelError</code>	A list giving the model error.
<code>optimizer</code>	A string giving the name of the optimization algorithm being used.
<code>optimizerParameters</code>	A list giving the parameters of the optimization algorithm.
<code>outputs</code>	A list giving the model outputs.
<code>designs</code>	A list giving the designs to be evaluated.
<code>fimType</code>	A string giving the type of Fim being evaluated.
<code>fim</code>	A object Fim giving the Fim.
<code>odeSolverParameters</code>	A list giving the atol and rtol parameters for the ode solver.
<code>optimisationDesign</code>	A list giving the evaluation of initial and optimal design.

optimisationAlgorithmOutputs	A list giving the outputs of the optimization process.
N	A numeric giving the parameter N.
muteEffect	A numeric giving the parameter muteEffect.
maxIteration	A numeric giving the parameter maxIteration.
purgeIteration	A numeric giving the parameter purgeIteration.
seed	A numeric giving the parameter seed.
showProcess	A Boolean giving showProcess.

plotEvaluation	<i>plotEvaluation: plots for the evaluation of the model responses.</i>
----------------	---

Description

plotEvaluation: plots for the evaluation of the model responses.

Arguments

pfimproject	A object PFIMProject.
plotOptions	A list giving the plot options.

Value

All the plots for the evaluation of the model responses.

plotEvaluationResults	<i>plotEvaluationResults: process for the evaluation of the responses.</i>
-----------------------	--

Description

plotEvaluationResults: process for the evaluation of the responses.

Arguments

arm	A object of class Arm giving the arm.
evaluationModel	A list giving the evaluation of the model.
outputNames	A list of string giving the output of the evaluation of the model.
samplingData	A list giving the sampling data from the method getSamplingData.
unitXAxis	A list giving the unit of the x-axis.
unitYAxis	A list giving the unit of the y-axis.
designName	A string giving the design name.

Value

A list giving the plot of the evaluation of the model responses.

plotEvaluationSI	<i>plotEvaluationSI: process for the evaluation of the gradient of the responses.</i>
------------------	---

Description

plotEvaluationSI: process for the evaluation of the gradient of the responses.

Arguments

arm	A object of class Arm giving the arm.
evaluationModelGradient	A list giving the evaluation of the gradient of the model responses.
parametersNames	A vector of string giving the parameter names?
outputNames	A list of string giving the name of the outputs.
samplingData	A list giving the sampling data from the method getSamplingData.
unitXAxis	A list giving the unit of the x-axis.
unitYAxis	A list giving the unit of the y-axis.
designName	A string giving the design name.

Value

A list giving the plot of the evaluation of gradient of the model responses.

plotFrequencies	<i>Plot frequencies for the FedorovWynn algorithm</i>
-----------------	---

Description

Plot frequencies for the FedorovWynn algorithm

Arguments

optimization	An Optimization object.
--------------	-------------------------

Value

Graph of the optimal frequencies.

plotFrequenciesFedorovWynnAlgorithm
<i>plotFrequenciesFedorovWynnAlgorithm</i>

Description

plotFrequenciesFedorovWynnAlgorithm

Arguments

optimization optimization
optimizationAlgorithm
 optimizationAlgorithm

Value

plotFrequenciesFedorovWynnAlgorithm

plotRSE	<i>Plot relative standard errors</i>
---------	--------------------------------------

Description

Plot relative standard errors
plotRSE: bar plot of the RSE.

Arguments

optimization An Optimization object.
pfimproject A object PFIMProject giving the Evaluation.

Value

Graph of relative standard errors
The bar plot of the RSE.

plotRSEFIM	<i>plotRSEFIM: barplot for the RSE</i>
------------	--

Description

plotRSEFIM: barplot for the RSE
plotRSEFIM: barplot for the RSE
plotRSEFIM: barplot for the RSE

Arguments

fim An object PopulationFim giving the Fim.
evaluation An object Evaluation giving the evaluation of the model.

Value

The bar plot of the RSE.
The bar plot of the RSE.
The bar plot of the RSE.

plotSE	<i>Plot standard errors</i>
--------	-----------------------------

Description

Plot standard errors
plotSE: bar plot of the SE.

Arguments

optimization An Optimization object.
pfimproject A object PFIMProject giving the Evaluation.

Value

Graph of standard errors
The bar plot of the SE.

plotSEFIM	<i>plotSEFIM: barplot for the SE</i>
-----------	--------------------------------------

Description

plotSEFIM: barplot for the SE

plotSEFIM: barplot for the SE

plotSEFIM: barplot for the SE

Arguments

fim An object PopulationFim giving the Fim.

evaluation An object Evaluation giving the evaluation of the model.

Value

The bar plot of the SE.

The bar plot of the SE.

The bar plot of the SE.

plotSensitivityIndices	<i>Plot sensitivity indices.</i>
------------------------	----------------------------------

Description

Plot sensitivity indices.

plotSensitivityIndices: plots for the evaluation of the gradient of the model responses.

Arguments

optimization An Optimization object.

pfimproject A object PFIMProject giving the Evaluation.

plotOptions A list giving the plot options.

Value

Graph of sensitivity indices.

All the plots for the evaluation of the gradient of the model responses.

plotShrinkage	<i>plotShrinkage: plot the shrinkage values.</i>
---------------	--

Description

plotShrinkage: plot the shrinkage values.

Arguments

- fim An object BayesianFim giving the Fim.
- evaluation An object Evaluation giving the evaluation of the model.

Value

The bar plot of the shrinkage.

plotWeights	<i>Plot weights for the multiplicative algorithm</i>
-------------	--

Description

Plot weights for the multiplicative algorithm

Arguments

- optimization An Optimization object.

Value

Plot of weights

plotWeightsMultiplicativeAlgorithm	<i>plotWeightsMultiplicativeAlgorithm: plot the optimal weight.</i>
------------------------------------	---

Description

plotWeightsMultiplicativeAlgorithm: plot the optimal weight.

Arguments

- optimization A object Optimization.
- optimizationAlgorithm A object MultiplicativeAlgorithm.

Value

The graph plotWeight.

PopulationFim	<i>PopulationFim</i>
---------------	----------------------

Description

The class PopulationFim represents and stores information for the PopulationFim.

Usage

```
PopulationFim(  
  fisherMatrix = numeric(0),  
  fixedEffects = numeric(0),  
  varianceEffects = numeric(0),  
  SEAndRSE = list(),  
  condNumberFixedEffects = 0,  
  condNumberVarianceEffects = 0,  
  shrinkage = numeric(0)  
)
```

Arguments

- fisherMatrix A matrix giving the numerical values of the Fim.
- fixedEffects A matrix giving the numerical values of the fixedEffects of the Fim.
- varianceEffects A matrix giving the numerical values of varianceEffects of the Fim.
- SEAndRSE A data frame giving the value of the SE and RSE.
- condNumberFixedEffects The conditional number of the fixedEffects of the Fim.
- condNumberVarianceEffects The conditional number of the varianceEffects of the Fim.
- shrinkage A vector giving the shrinkage values.

`processArmEvaluationResults`*processArmEvaluationResults: process for the evaluation of an arm.*

Description

`processArmEvaluationResults`: process for the evaluation of an arm.

Arguments

<code>arm</code>	A object of class <code>Arm</code> giving the arm.
<code>model</code>	A object of class <code>Model</code> giving the model.
<code>fim</code>	A object of class <code>Fim</code> giving the fim.
<code>designName</code>	A string giving the name of the design.
<code>plotOptions</code>	A list giving the plot options.

Value

A list of ggplot object giving the plot of the responses ans the gradient responses of the the model.

`processArmEvaluationSI`*processArmEvaluationSI: process for the evaluation of the gradient of the responses.*

Description

`processArmEvaluationSI`: process for the evaluation of the gradient of the responses.

Arguments

<code>arm</code>	A object of class <code>Arm</code> giving the arm.
<code>model</code>	A object of class <code>Model</code> giving the model.
<code>fim</code>	A object of class <code>Fim</code> giving the fim.
<code>designName</code>	A string giving the name of the design.

Value

A list giving the ggplot object of the plots of the gradient.

Proportional

Proportional

Description

The class `Proportional` is used to defined a model error.

Usage

```
Proportional(
    output = character(0),
    equation = expression(sigmaSlope),
    derivatives = list(),
    sigmaInter = 0,
    sigmaSlope = 0,
    sigmaInterFixed = FALSE,
    sigmaSlopeFixed = FALSE,
    cError = 1
)
```

Arguments

<code>output</code>	A string giving the model error output.
<code>equation</code>	A expression giving the model error equation.
<code>derivatives</code>	A list giving the derivatives of the model error equation.
<code>sigmaInter</code>	A double giving the sigma inter.
<code>sigmaSlope</code>	A double giving the sigma slope
<code>sigmaInterFixed</code>	A Boolean giving if the sigma inter is fixed or not. - not in the v7.0
<code>sigmaSlopeFixed</code>	A Boolean giving if the sigma slope is fixed or not. - not in the v7.0
<code>cError</code>	A integer giving the power parameter.

PSOAlgorithm

PSOAlgorithm

Description

The class `PSOAlgorithm` implements the PSO algorithm.

Usage

```

PSOAlgorithm(
  name = character(0),
  modelEquations = list(),
  modelFromLibrary = list(),
  modelParameters = list(),
  modelError = list(),
  optimizer = character(0),
  optimizerParameters = list(),
  outputs = list(),
  designs = list(),
  fimType = character(0),
  fim = Fim(),
  odeSolverParameters = list(),
  optimisationDesign = list(),
  optimisationAlgorithmOutputs = list(),
  maxIteration = numeric(0),
  populationSize = numeric(0),
  seed = numeric(0),
  personalLearningCoefficient = numeric(0),
  globalLearningCoefficient = numeric(0),
  showProcess = FALSE
)

```

Arguments

<code>name</code>	A string giving the name of the design evaluation.
<code>modelEquations</code>	A list giving the model equations.
<code>modelFromLibrary</code>	A list giving the model equations from the library of model.
<code>modelParameters</code>	A list giving the model parameters.
<code>modelError</code>	A list giving the model error.
<code>optimizer</code>	A string giving the name of the optimization algorithm being used.
<code>optimizerParameters</code>	A list giving the parameters of the optimization algorithm.
<code>outputs</code>	A list giving the model outputs.
<code>designs</code>	A list giving the designs to be evaluated.
<code>fimType</code>	A string giving the type of Fim being evaluated.
<code>fim</code>	A object Fim giving the Fim.
<code>odeSolverParameters</code>	A list giving the atol and rtol parameters for the ode solver.
<code>optimisationDesign</code>	A list giving the evaluation of initial and optimal design.

optimisationAlgorithmOutputs	A list giving the outputs of the optimization process.
maxIteration	A numeric giving the maxIteration.
populationSize	A numeric giving the populationSize.
seed	A numeric giving the seed.
personalLearningCoefficient	A numeric giving the personalLearningCoefficient.
globalLearningCoefficient	A numeric giving the globalLearningCoefficient.
showProcess	A Boolean giving the showProcess.

replaceVariablesLibraryOfModels

replaceVariablesLibraryOfModels: replace variable in the LibraryOf-Models

Description

replaceVariablesLibraryOfModels: replace variable in the LibraryOfModels

Usage

```
replaceVariablesLibraryOfModels(text, old, new)
```

Arguments

text	the text
old	old string
new	new string

Value

text with new string

Report	<i>Generate optimization report</i>
--------	-------------------------------------

Description

Generate optimization report

Report: generate the report.

Arguments

optimization	An Optimization object.
pfimproject	A object PFIMProject giving the Evaluation or Optimization.
outputPath	A string giving the path where the output are saved.
outputFile	A string giving the name of the output file.
plotOptions	A list giving the plot options.

Value

Generated report.

The html report of the design evaluation or optimization.

run	<i>Run optimization</i>
-----	-------------------------

Description

Run optimization

run: run the evaluation of a design.

Arguments

optimization	An Optimization object.
pfimproject	A object PFIMProject giving the Evaluation.

Value

The optimization design results.

The object Evaluation giving the design evaluation.

SamplingTimeConstraints

SamplingTimeConstraints

Description

The class "SamplingTimeConstraints" implements the constraints for the sampling times.

Usage

```
SamplingTimeConstraints(
  outcome = character(0),
  initialSamplings = 0,
  fixedTimes = 0,
  numberOfsamplingsOptimisable = 0,
  samplingsWindows = list(),
  numberOfTimesByWindows = 0,
  minSampling = 0
)
```

Arguments

outcome	A string giving the outcome.
initialSamplings	A vector of numeric giving the initialSamplings.
fixedTimes	A vector of numeric giving the fixedTimes.
numberOfsamplingsOptimisable	A vector of numeric giving the numberOfsamplingsOptimisable.
samplingsWindows	A vector of numeric giving the samplingsWindows.
numberOfTimesByWindows	A vector of numeric giving the numberOfTimesByWindows.
minSampling	A vector of numeric giving the minSampling.

SamplingTimes

SamplingTimes

Description

The class SamplingTimes is used to defined SamplingTimes.

Usage

```
SamplingTimes(outcome = character(0), samplings = numeric(0))
```


Arguments

fim An object PopulationFim giving the Fim.
 optimizationAlgorithm An object FedorovWynnAlgorithm giving the optimization algorithm.

Value

The optimal arms.
 The optimal arms.
 The list optimalArms.
 The list optimalArms.
 The list optimalArms.
 The list optimalArms.

setSamplingConstraintForOptimization

setSamplingConstraintForOptimization: set the sampling time constraints for an arm for the design optimization.

Description

setSamplingConstraintForOptimization: set the sampling time constraints for an arm for the design optimization.

Arguments

design An object Design giving the design.

Value

The arm with the sampling time constraint for the design optimization.

show

Show optimization results

Description

Show optimization results
 show: show the evaluation in the R console.

Arguments

optimization An Optimization object.
 pfimproject A object PFIMProject giving the Evaluation.

Value

Prints results to console.
The show of the evaluation of the design.

showFIM	<i>showFIM: show the Fim in the R console.</i>
---------	--

Description

showFIM: show the Fim in the R console.
showFIM: show the Fim in the R console.
showFIM: show the Fim in the R console.

Arguments

fim An object IndividualFim giving the Fim.

Value

The fisherMatrix, fixedEffects, Determinant, condition numbers and D-criterion, Shrinkage and Parameters estimation
The fisherMatrix, fixedEffects, Determinant, condition numbers and D-criterion, Shrinkage and Parameters estimation
The fisherMatrix, fixedEffects, Determinant, condition numbers and D-criterion, Shrinkage and Parameters estimation

SimplexAlgorithm	<i>SimplexAlgorithm</i>
------------------	-------------------------

Description

The class SimplexAlgorithm implements the Simplex algorithm.

Usage

```
SimplexAlgorithm(  
  name = character(0),  
  modelEquations = list(),  
  modelFromLibrary = list(),  
  modelParameters = list(),  
  modelError = list(),  
  optimizer = character(0),  
  optimizerParameters = list(),  
  outputs = list(),
```



```

    designs = list(),
    fimType = character(0),
    fim = Fim(),
    odeSolverParameters = list(),
    optimisationDesign = list(),
    optimisationAlgorithmOutputs = list(),
    pctInitialSimplexBuilding = numeric(0),
    maxIteration = numeric(0),
    seed = numeric(0),
    tolerance = numeric(0),
    showProcess = FALSE
)

```

Arguments

name	A string giving the name of the design evaluation.
modelEquations	A list giving the model equations.
modelFromLibrary	A list giving the model equations from the library of model.
modelParameters	A list giving the model parameters.
modelError	A list giving the model error.
optimizer	A string giving the name of the optimization algorithm being used.
optimizerParameters	A list giving the parameters of the optimization algorithm.
outputs	A list giving the model outputs.
designs	A list giving the designs to be evaluated.
fimType	A string giving the type of Fim being evaluated.
fim	A object Fim giving the Fim.
odeSolverParameters	A list giving the atol and rtol parameters for the ode solver.
optimisationDesign	A list giving the evaluation of initial and optimal design.
optimisationAlgorithmOutputs	A list giving the outputs of the optimization process.
pctInitialSimplexBuilding	A numeric giving the pctInitialSimplexBuilding.
maxIteration	A numeric giving the maxIteration.
seed	A numeric giving the seed.
tolerance	A numeric giving the tolerance.
showProcess	A Boolean giving the showProcess.

tablesForReport	<i>tablesForReport: generate the table for the report.</i>
-----------------	--

Description

tablesForReport: generate the table for the report.

tablesForReport: generate the table for the report.

tablesForReport: generate the table for the report.

Arguments

fim An object PopulationFim giving the Fim.

evaluation An object Evaluation giving the evaluation of the model.

Value

fixedEffectsTable, FIMCriteriaTable, SEAndRSETable.

fixedEffectsTable, FIMCriteriaTable, SEAndRSETable.

fixedEffectsTable, FIMCriteriaTable, SEAndRSETable.

updateSamplingTimes	<i>updateSamplingTimes: update sampling times for plotting used for plot</i>
---------------------	--

Description

updateSamplingTimes: update sampling times for plotting used for plot

Arguments

arm A object of class Arm giving the arm.

samplingData The list giving as output in the method getSamplingData.

Value

The updated sampling times.

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